

**SAO PARTICIPATION IN THE GOME AND SCIAMACHY
SATELLITE INSTRUMENTS PROGRAMS**

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Principal Investigator
Kelly Chance

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SMITHSONIAN INSTITUTION
ASTROPHYSICAL OBSERVATORY
CAMBRIDGE, MASSACHUSETTS 02138

Director: Irwin I. Shapiro

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is a member of the
Harvard-Smithsonian Center for Astrophysics

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Progress as of June 30, 2003

Principal Investigator

Dr. Kelly Chance

Co-Investigator

Dr. Thomas Kurosu

1. Introduction

This report summarizes the progress on our three-year program of research to refine the measurement capability for satellite-based instruments that monitor ozone and other trace species in the Earth's stratosphere and troposphere, to retrieve global distributions of these and other constituents from the GOME and SCIAMACHY satellite instruments, and to conduct scientific studies for the ILAS instruments. This continues our involvements as a U.S. participant in GOME and SCIAMACHY since their inception, and as a member of the ILAS-II Science Team. These programs have led to the launch of the first satellite instrument specifically designed to measure height-resolved ozone, including the tropospheric component (GOME), and the development of the first satellite instrument that will measure tropospheric ozone simultaneously with NO₂, CO, HCHO, N₂O, H₂O, and CH₄ (SCIAMACHY). The GOME program now includes the GOME-2 instruments, to be launched on the Eumetsat Metop satellites, providing long-term continuity in European measurements of global ozone that complement the measurements of the TOMS, SBUV, OMI, OMPS instruments.

The research primarily focuses on two areas: *Data analysis*, including algorithm development and validation studies that will improve the quality of retrieved data products, in support for future field campaigns (to complement in situ and airborne campaigns with satellite measurements), and *scientific analyses* to be interfaced to atmospheric modeling studies.

2. Progress in First Year of Studies

2.1 SCIAMACHY

The SCIAMACHY instrument was launched on the Envisat satellite on March 1, 2002. At present, SCIAMACHY is still in the process of verification and early validation. No operational products have yet been released. We have been working with the European Space Agency, as head of the SCIAMACHY Algorithm Development and Data Usage

subgroup (SADDU) of the SCIAMACHY Science Advisory Group (SSAG) and the German Aerospace Center (DLR) to optimize the operational algorithms for validation and eventual data product release.

2.1.1 Algorithm studies

Cloud correction

The impact of clouds for limb scattering geometry is handled by using a high tangent height reference. For middle stratospheric tangent heights (TH), the cloud signature is nearly identical to the cloud signature of the high tangent height reference. Thus, after high tangent height normalization, the impact of clouds is considerably reduced. In the lower stratosphere (TH < 20 km), the cloud signature increases monotonically down to the cloud top. At $z=19$ km, this simple and indirect method of cloud correction reduces NO₂ number density errors due to cloud neglect in the forward model to <1%, 2.5%, 7%, 11% at solar zenith angles of 89, 79, 57, and 30°. The error due to clouds increases at small solar zenith angles because the incoming solar radiation can penetrate more deeply and reflects more squarely off the plane-parallel cloud top than at grazing incidences. This study assumed an optically thick cloud deck with top at 3 km and base at 0.66 km and extinction of 92.6 km⁻¹ (at $\lambda = 550$ nm).

Wavelength calibration

The wavelength calibration method using cross-correlation with a high-resolution Fraunhofer spectrum we introduced for GOME [Caspar and Chance, 1997] is fully implemented for SCIAMACHY, for use as a backup for wavelength calibration in case the line calibration lamp fails.

We have taken a standard ATMOS solar reference spectrum, which covers the SCIAMACHY Channel 8 (infrared; CO and N₂O channel), recalibrated it in absolute wavelength to 0.002 cm⁻¹ (0.001 nm, or 0.01 SCIAMACHY pixel) using solar CO lines, and supplied it with software to convolve to SCIAMACHY spectral resolution. This solar spectrum will be used in wavelength calibration as well as for determining undersampling in this SCIAMACHY channel (see **Spectral and spatial sampling tests**, below) and to improve the slit function determination as was done previously in the UV-visible (see above references).

Spectral and spatial sampling tests

We initially determined the undersampling correction for the GOME instrument [Chance, 1998] and, with DLR colleagues, improved it for application to SCIAMACHY [Slijkhuis *et al.*, 1999].

We are in the process of conducting a rigorous analytical study of spectral undersampling which will apply directly to SCIAMACHY, the GOME instruments, OMI, and OMPS

(and, presumably, other instruments as well). This will improve the correction for undersampling for all of these instruments, and put it on a firmer theoretical basis.

Ring effect studies

We have supplied Ring effect correction spectra to the DLR for use in operational processing of both limb and nadir spectra.

If a high TH reference spectrum is used in limb processing, the Ring effect cancels out to a very good approximation. Co-adding many high TH spectra at a variety of temperatures minimizes the residual Ring effect due to the temperature dependence of the rotational Raman scattering. Using a single high TH spectrum near the stratopause has been shown to increase fitting residuals because the stratopause is much warmer than the lower stratosphere and thus the Ring effect signature is spectrally different. It was found that the residual Ring effect structure after high TH normalization is apparently a function of line shape as well as line depth. An example is the Fraunhofer line at 351.45 nm, which tends to exhibit large residual Ring effect structures relative to other lines in the 345-360 nm window in both SCIAMACHY and simulated spectra, despite being a relatively weak line.

Database improvement

We have supplied improved reference spectra to the DLR for use in operation processing, including O₃ [Orphal and Chance, 2003; Rinsland *et al.*, 2003] and SO₂ [Rufus *et al.*, 2003]. Temperature-dependent cross sections are derived from the Bass-Paur measurements, with improved absolute wavelength calibration; they have been supplied at SCIAMACHY resolution.

We have made a full set of recommendations for UV /visible cross sections to be included in HITRAN, and are in the process of implementing them [Orphal and Chance, 2003; Rothman *et al.*, 2003].

2.1.2 Scientific studies

We have provided recommendations to the DLR for the SCIAMACHY level 1-2 processing baseline and have performed studies to optimize the operational processing algorithm for several species, including HCHO (in progress), limb NO₂ (complete), limb BrO (complete), and limb OCIO (in progress).

We have implemented improved methods to determine limb pointing, by using comparisons of measured and modeled “knees” in the limb scattered light, including the use of multiple knees at different wavelengths, and the knee at 305 nm [Sioris *et al.*, 2003]. These approaches have been found to identify and correct for inaccurate pointing information supplied by the satellite to on the order of 400 meters.

We have started preliminary studies (under separate funding) to develop tropospheric data products from SCIAMACHY. We have retrieved tropospheric NO₂ with the limb-nadir matching technique. The stratospheric (and occasionally upper tropospheric) NO₂ profile is retrieved down to:

1. cloud top, or
2. the vertical (2-km) layer below which the uncertainty of the integrated vertical profile above due to including the underlying layer is larger than the resulting increase to the vertical column density.

The profile retrieval range is typically 15-41 km. Large columns have been detected over various urban centers such as Los Angeles. Individual power plants in remote areas have been detected with the 30 km × 60 km spatial resolution of nadir geometry (assuming the stratospheric NO₂ does not vary appreciably over such short spatial scales outside the polar vortex). A high bias at high northern latitudes and a low bias in the tropics have been detected by limb-nadir matching when the total column from the operational NO₂ product is used, confirming the same finding from research groups at other institutions.

Tropospheric HCHO determinations are lagging, compared to those from our work on GOME data, because of the need to fully implement improved characterization of the polarization sensitivity into the Level 0-1 algorithm, but this is expected to be completed by September 2003.

2.2 GOME-2 Studies

Fraunhofer cross-correlation has been implemented for operational wavelength calibration, as the backup in case the line calibration lamp fails.

We have performed detailed intercomparisons of alternate trace gas slant column fitting techniques, and the use of alternate reference spectra for GOME. The basic result is that the use of direct ("BOAS") fitting of the measured radiances provides better fitting results (lower fitting uncertainties and better correlation with TOMS measurements) than fitting to the high-pass filtered logarithm of the ratio of the radiance to the irradiance ("DOAS").

We have also found that the use of the Bass-Paur ozone cross sections with improved wavelength calibration [Orphal and Chance, 2003], convolved to GOME resolution, provides better ozone fitting results than those obtained with the use of the GOME-FM cross sections.

2.3 ILAS

The PSC detection method developed for ILAS is now mature for occultation viewing mode. Based on thresholds derived from ILAS measurements, likely PSC events are

identified from enhanced stratospheric aerosol optical thickness in the altitude range of ~20-30 km.

The next steps include the application of the technique to ILAS-II and SCIAMACHY occultation data (neither of which are currently available). This will determine whether thresholds on optical thickness derived from one sensor can be generalized and applied to observations from other instruments. Furthermore, we plan to adopt the method to limb viewing geometry, where a PSC shows up as an enhanced scattering event rather than a reduction in transmittance.

3. Schedule for Second and Third Years

3.1 Second year

SCIAMACHY Studies

Algorithm studies

- Cloud correction
- Ring effect studies

Scientific studies

- Tropospheric NO₂, HCHO, CO, CH₄, CO₂, and N₂O
- Polar stratospheric cloud measurements

Ongoing GOME-2 studies

Ongoing ILAS-II studies

3.2 Third year

SCIAMACHY Studies

Scientific studies

- Tropospheric NO₂, HCHO, CO, CH₄, CO₂, and N₂O
- Polar stratospheric cloud measurements

Ongoing GOME-2 studies

Ongoing ILAS-II studies

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